Benzamide, 2,6-difluoro-3-methyl-N-decyl-

Inchi: InChI=1S/C18H27F2NO/c1-3-4-5-6-7-8-9-10-13-21-18(22)16-15(19)12-11-14(2)17(16)20
InchiKey: XBWJBDDZMJTVOP-UHFFFAOYSA-N
Formula: C18H27F2NO
SMILES: CCCCCCCCCCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 311.41

Physical Properties

Property code	Value	Unit	Source
gf	-244.95	kJ/mol	Joback Method
hf	-664.06	kJ/mol	Joback Method
hfus	48.11	kJ/mol	Joback Method
hvap	71.47	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.144		Crippen Method
mcvol	255.810	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	755.44	K	Joback Method
tc	941.72	K	Joback Method
tf	460.37	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.06	J/mol×K	755.44	Joback Method
cpg	772.12	J/mol×K	786.49	Joback Method
cpg	787.30	J/mol×K	817.53	Joback Method
cpg	801.64	J/mol×K	848.58	Joback Method
cpg	815.15	J/mol×K	879.63	Joback Method
cpg	827.88	J/mol×K	910.68	Joback Method
cpg	839.85	J/mol×K	941.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407746&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume